Supplementary Information

Production and Characterization of the Bio-Oil Obtained by the Fast Pyrolysis of Spent Coffee Grounds of the Soluble Coffee Industry

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Table S1. Identified compounds in bio-oil (by GC-MS), according to Figure 5 of the main text

Peak number	Name	t_R / min	Area / %	LPTRI[a]		
				Experimental	NIST	ΔRI[b]
4	pentanoic acid	16.78	0.66	888	894	–6
7	pentanoic acid, 4-methyl-	20.39	1.19	957	949	8
47	nonanoic acid	36.24	0.27	1.271	1.272	–1
99	n-hexadecanoic acid	63.74	13.96	1.976	1.976	0
106	9,12-octadecadienoic acid (*Z*,*Z*)-	69.15	9.40	2.151	2.146	5
107	octadecanoic acid	69.79	4.94	2.173	2.173	0
Acids (6 peaks)			30.43			
3	2-furanmethanol	15.35	1.23	861	863	–2
83	2-tetradecen-1-ol	53.04	0.16	1.668	1.664	4
84	*cis*-7-tetradecen-1-ol	53.18	0.31	1.672	1.660	12
85	1-tetradecanol	53.45	0.52	1.679	1.679	0
97	2-heptadecanol	61.38	0.79	1.903	1.909	–6
Alcohols (5 peaks)			3.01			
67	benzoic acid, 4-hydroxy-, methyl ester	43.56	0.47	1.439	1.452	–13
98	hexadecanoic acid, methyl ester	62.09	0.84	1.925	1.925	0
102	9-octadecenoic acid (*Z*)-, methyl ester	66.89	2.47	2.076	2.082	–6
103	9,12-octadecadienoic acid (*Z*,*Z*)-, methyl ester	67.51	0.66	2.096	2.096	0
105	octadecanoic acid, methyl ester	68.44	0.78	2.127	2.127	0
111	octadecanoic acid, 2-propenyl ester	72.78	0.61	2.268	2.251	17
113	eicosanoic acid, methyl ester	74.22	1.16	2.329	2.329	0
Esters (7 peaks)			6.99			

Table S1. Identified compounds in bio-oil (by GC-MS), according to Figure 5 of the main text (cont.)

Peak number	Name	t_R / min	Area / %	LPTRI[a]		
				Experimental	NIST	ΔRI[b]
40	benzofuran, 4,7-dimethyl-	34.18	0.17	1.228	1.220	8
43	benzene, 2-methoxy-1-isoproyl,4-methyl	34.90	0.30	1.243	1.236	7
51	3,5-dimethoxytoluene	37.02	0.27	1.287	1.270	17
70	(4-methylphenyl) methanol, *n*-pentyl ether	45.53	0.21	1.479	1.464	15
Ethers (4 peaks)			0.96			
19	benzene, butyl-	25.85	0.08	1.062	1.058	4
33	benzene, pentyl-	31.04	0.16	1.164	1.160	4
46	benzene, hexyl-	36.07	0.41	1.267	1.261	6
48	benzene, pentamethyl	36.36	0.21	1.273	1.287	–14
60	benzene, 1-butyl,2,4,6-trimethyl	40.87	0.63	1.371	1368	3
61	benzene, heptyl-	41.05	0.24	1.375	1.369	6
69	benzene, octyl-	45.36	0.33	1.475	1.468	7
78	benzene, nonyl-	49.62	0.51	1.579	1.586	–7
89	benzene, C11	54.42	0.31	1.704	n.f.	
90	benzene, C11	54.73	0.22	1.713	n.f.	
91	benzene, undecyl-	57.42	0.48	1.788	1.780	8
57	naphthalene, 1-methyl-	38.24	0.23	1.313	1.299	14
59	naphthalene, 2-methyl-	39.01	0.16	1.330	1.316	14
66	naphthalene, 1,3-dimethyl-	42.68	0.38	1.412	1.409	3
68	naphthalene, 1,5-dimethyl-	43.81	0.28	1.438	1.438	0
76	germacrene D	47.27	0.25	1.521	1.520	1
12	2,6-dimethyl-2,6-octadiene	22.74	0.17	1.002	990	12
17	1,5-heptadiene, 2,3,6-trimethyl-	25.08	0.09	1.047	1.063	–16

Table S1. Identified compounds in bio-oil (by GC-MS), according to Figure 5 of the main text (cont.)

Peak number	Name	t_R / min	Area / %	LPTRI[a]		
				Experimental	NIST	ΔRI[b]
52	1-tridecene	37.30	0.29	1.293	1.293	0
63	1-tetradecene	41.84	0.70	1.393	1.393	0
71	1-pentadecene	46.12	0.56	1.493	1.492	1
74	2-pentadecene (E)	46.61	0.47	1.504	1.507	–3
75	2-pentadecene	47.09	0.23	1.516	1.517	–1
79	1-hexadecene	49.86	0.38	1.585	1.587	–2
80	3-hexadecene	50.16	0.50	1.592	1.604	–12
82	2-hexadecene	50.60	0.30	1.604	1.618	–14
86	1-heptadecene	53.63	0.92	1.683	1.682	1
87	8-heptadecene	53.98	0.38	1.692	1.704	–12
93	1-hexadecene, 7,11,15-trimethyl-3-methylene	59.12	0.45	1.837	1.837	0
95	1-nonadecene	61.04	0.36	1.893	1.892	1
115	squalene	86.49	0.20	2.819	2.836	–17
54	tridecane	37.68	0.35	1.301	1.300	1
64	tetradecane	42.19	1.02	1.401	1.400	1
73	pentadecane	46.46	1.78	1.500	1.500	0
81	hexadecane	50.44	0.51	1.599	1.600	–1
88	heptadecane	54.24	0.91	1.699	1.700	–1
92	octadecane	57.83	0.30	1.799	1.800	–1
96	nonadecane	61.25	0.52	1.899	1.900	–1
100	eicosane	64.52	2.10	2.000	2.000	0
104	heneicosane	67.62	0.88	2.100	2.100	0
109	docosane	70.60	1.68	2.200	2.200	0

Table S1. Identified compounds in bio-oil (by GC-MS), according to Figure 5 of the main text (cont.)

Peak number	Name	t_R / min	Area / %	LPTRI[a]		
				Experimental	NIST	ΔRI[b]
112	tricosane	73.42	0.60	2.299	2.300	–1
Hydrocarbons (42 peaks)	21.51					
2	2-cyclopenten-1-one	14.54	0.74	845	835	10
5	2-cyclopenten-1-one, 2-methyl-	17.98	0.52	911	910	1
6	ethanone, 1-(2-furanyl)-	18.15	0.37	914	914	0
8	2-butanone, 4-(acetyloxy)-	20.71	0.13	968	985	–17
9	2-cyclopenten-1-one, 3-methyl-	21.13	0.52	972	973	–1
11	cyclopentenone, dimethyl-	22.59	0.34	1.000	n.f.	
14	1,2-cyclopentanedione, 3-methyl-	24.27	1.18	1.032	1.043	–11
15	2-acetyl-5-methylfuran	24.62	0.18	1.038	1.042	–4
16	2-cyclopenten-1-one, 2,3-dimethyl-	24.84	0.31	1.043	1.040	3
20	2-cyclopenten-1-one, 2,3,4-trimethyl-	26.06	0.12	1.066	1071	–5
21	ethanone, 1-(1*H*-pyrrol-2-yl)-	26.26	0.18	1.070	1.072	–2
22	acetophenone	26.49	0.19	1.074	1.075	–1
24	bicyclo[3.1.0]hexan-3-one, 4-methyl-1-(1-methylethyl)-	26.97	0.28	1.084	1.100	–16
27	maltol	28.79	0.62	1.119	1.114	5
28	2-cyclopenten-1-one, 3-ethyl-2-hydroxy-	29.02	0.32	1.124	1.140	–16
39	hydroxy-C3-cyclopentenone	33.52	0.25	1.214	n.f.	
53	1*H*-inden-1-one, 2,3-dihydro-	37.44	0.53	1.296	1.292	4
65	indanone, methyl-	42.55	0.15	1.409	n.f.	
Ketones (18 peaks)			6.93			

Table S1. Identified compounds in bio-oil (by GC-MS), according to Figure 5 of the main text (cont.)

Peak number	Name	t_R / min	Area / %	LPTRI[a]		
				Experimental	NIST	ΔRI[b]
1	pyridine	11.21	2.89	781	769	12
13	pyrazine, 2-ethyl-5-methyl-	22.85	0.05	1.005	1.006	–1
30	benzyl nitrile	30.13	0.19	1.146	1.145	1
36	1*H*-pyrrole, 1-(2-furanylmethyl)-	32.12	0.10	1.185	1.185	0
55	indole	37.92	0.35	1.306	1.300	6
72	indole, 2,3-dimethyl-	46.27	0.33	1.496	1.499	–3
77	indole, c3	49.29	0.25	1.571	n.f.	
94	caffeine	60.29	3.47	1.861	1.848	13
101	9h-pyrido[3,4-*b*]indole	65.29	0.82	2.025	2.009	16
108	hexadecanamide	70.38	1.85	2.193	2.182	11
110	myristamide, *N*-isobutyl-	71.29	1.69	2.224	2.215	9
114	octadecanamide	76.07	0.58	2.396	2.398	–2
N-compounds (12 peaks)			12.55			
10	phenol	21.73	3.72	983	981	2
18	phenol, 2-methyl-	25.59	1.06	1.057	1.055	2
23	*p*-cresol	26.73	2.32	1.079	1.079	0
25	phenol, 2-methoxy-	27.46	0.70	1.093	1.092	1
26	phenol, 2,6-dimethyl-	28.54	0.34	1.114	1.114	0
29	phenol, 2-ethyl-	29.88	0.27	1.141	1.138	3
31	phenol, 2,4-dimethyl-	30.50	0.58	1.153	1.151	2
32	phenol, 2,5-dimethyl-	30.61	0.25	1.155	1.154	2

Table S1. Identified compounds in bio-oil (by GC-MS), according to Figure 5 of the main text (cont.)

Peak number	Name	RT / min	Area / %	LPTRI[a]		
				Experimental	NIST	ΔRI[b]
34	phenol, 4-ethyl-	31.39	1.46	1.171	1.168	3
35	phenol, 2,3-dimethyl-	31.99	0.31	1.183	1.184	–1
37	phenol, 2-methoxy-4-methyl	32.70	0.29	1.197	1.196	2
38	1,2-benzenediol (catechol)	32.98	2.16	1.202	1.200	2
41	phenol, 3-(1-methylethyl)	34.38	0.30	1.232	1.229	3
42	4-isopropylphenol	34.62	0.14	1.237	1.247	–10
44	phenol, 2,3,6-trimethyl	35.14	0.18	1.248	1.246	2
45	2-isopropyl-4-methylphenol	35.91	0.34	1.264	1262	2
49	phenol, 2,3,5-trimethyl-	36.45	0.25	1.275	1.275	0
50	phenol, 4-ethyl-2-methoxy-	36.84	1.72	1.283	1.282	1
56	phenol, 3,4,5-trimethyl-	38.08	0.12	1.310	1.320	–10
58	phenol, 2,3,5,6-tetramethyl-	38.59	0.61	1.321	1.319	2
62	1,3-benzenediol, 5-methyl (5-methyl-resorcinol)	41.73	0.52	1.390	1378	12
Phenols (21 peaks)			17.63			

[a]LPTRI: linear programmed temperature retention indexes; [b]$\Delta RI = LPTRI_{EXPERIMENTAL} - LPTRI_{NIST}$; n.f.: LPTRI not found, when the LPTRI were not found in the literature but the spectra is very similar (> 90%).